

L9 ANSWER 1 OF 7 CA COPYRIGHT 2003 ACS  
 AN 138:5819 CA  
 TI Selective alkylation of **catechol** with tert-butyl  
 alcohol over HY and modified HY **zeolites**  
 AU Anand, R.; Maheswari, R.; Gore, K. U.; Chumbhale, V. R.  
 CS Catalysis Division, National Chemical Laboratory, Pune, 411 008,  
 India  
 SO Catalysis Communications (2002), 3(8), 321-326  
 CODEN: CCAOAC; ISSN: 1566-7367  
 PB Elsevier Science B.V.  
 DT Journal  
 LA English  
 CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)  
 Section cross-reference(s): 67  
 AB Vapor phase alkylation of catechol with t-BuOH was studied over  
 HY and  
 dealuminated HY zeolites at 120-200.degree.C. The predominant  
 product is  
 4-tert-butylcatechol (4-TBC) with >86% selectivity; the minor  
 products are  
 3-tert-butylcatechol and 3,5-di-tert-butylcatechol.  
 Dealuminated HY  
 zeolites (steamed at 550.degree. and 700.degree.) showed marked  
 increase  
 in catechol conversion and 4-TBC yield. The effects of various  
 reaction  
 parameters, such as temp., space velocity and reactant molar  
 ratio are  
 discussed.  
 ST catechol butylation zeolite catalyst; butylcatechol prepn  
 catechol  
 butylation catalyst  
 IT Dealuminated Y zeolites  
 RL: CAT (Catalyst use); USES (Uses)  
 (HY; selective alkylation of catechol with t-BuOH over  
 dealuminated HY  
 zeolites)  
 IT Zeolite HY  
 RL: CAT (Catalyst use); USES (Uses)  
 (dealuminated; selective alkylation of catechol with t-BuOH  
 over  
 dealuminated HY zeolites)  
 IT Butylation catalysts  
 (selective alkylation of catechol with t-BuOH over  
 dealuminated HY  
 zeolites)  
 IT 98-29-3P, 4-tert-Butylcatechol  
 RL: IMF (Industrial manufacture); PREP (Preparation)  
 (prepn. by selective alkylation of catechol with t-BuOH over  
 dealuminated HY zeolites)

IT 75-65-0, tert-Butanol, reactions 120-80-9, Catechol, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(selective alkylation of catechol with t-BuOH over  
dealuminated HY zeolites)

RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD  
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L9 ANSWER 2 OF 7 CA COPYRIGHT 2003 ACS

AN 136:355704 CA

TI Alkylation of catechol with tert-butyl alcohol  
over H.beta. zeolite

AU Zhang, Jingchang; Sun, Faqun; Cao, Weiliang; Zhang, Tianqiao  
CS Faculty of Science, Beijing University of Chemical Technology,  
Beijing,  
100029, Peop. Rep. China

SO Cuihua Xuebao (2002), 23(1), 33-36  
CODEN: THHPD3; ISSN: 0253-9837

PB Kexue Chubanshe

DT Journal

LA Chinese

CC 37-2 (Plastics Manufacture and Processing)

AB Catalytic performance of H.beta. and modified H.beta./Al2O3 in  
alkylation

of catechol with tert-Bu alc. was investigated. The structure  
and acid

properties of the catalysts were characterized by XRD and NH3-TPD  
techniques. The influence of acidity of the zeolite on  
catalytic activity

and selectivity was discussed. The results showed that the  
selectivity of

Co-.beta./Al2O3 for 4-tert-butylcatechol reaches 99%, and the  
catechol

conversion is 71%, which is the best result reported in refs. up  
to date.

H.beta. zeolite and Co-modified H.beta./Al2O3 are prospective  
catalysts

for alkylation of catechol with t-Bu alc.

ST catechol butyl alc alkylation zeolite catalyst

IT Alkylation catalysts

(alkylation of catechol with tert-Bu alc. over H.beta. zeolite)

IT H-Beta zeolites

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);

USES (Uses)

(alkylation of catechol with tert-Bu alc. over H.beta. zeolite)

IT Beta zeolites

RL: RCT (Reactant); RACT (Reactant or reagent)

(alkylation of catechol with tert-Bu alc. over H.beta. zeolite)

IT 1344-28-1, Alumina, uses

RL: CAT (Catalyst use); USES (Uses)

(alkylation of catechol with tert-Bu alc. over H.beta. zeolite)

IT 75-65-0, tert-Butanol, reactions 120-80-9, O-Dihydroxybenzene, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(alkylation of catechol with tert-Bu alc. over H.beta. zeolite)

IT 98-29-3P, 4-Tert-Butyl-1,2-benzenediol

RL: SPN (Synthetic preparation); PREP (Preparation)

(alkylation of catechol with tert-Bu alc. over H.beta. zeolite)

L9 ANSWER 3 OF 7 CA COPYRIGHT 2003 ACS

AN 136:249325 CA

TI Alkylation of catechol with tert-butyl alcohol over modified Co.beta. zeolite

AU Zhang, Jing-chang; Sun, Fa-qun; Cao, Wei-liang

CS Faculty of Science, Beijing University of Chemical Technology, Beijing,

100029, Peop. Rep. China

SO Ningxia Daxue Xuebao, Ziran Kexueban (2001), 22(2), 109-111

CODEN: NDXKD8; ISSN: 0253-2328

PB Ningxia Daxue Xuebao, Ziran Kexueban Bianjibu

DT Journal

LA Chinese

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)

Section cross-reference(s): 67

AB Alkylation of catechol with t-BuOH over modified .beta. zeolites was

investigated. The pore structure and acid properties of catalysts were

characterized by XRD and NH3-TPD. The activity of Co.beta. zeolite is

high, the conversion of catechol is 71% and the selectivity to 4-tert-butylcatechol is 99%.

ST catechol alkylation butanol cobalt zeolite

catalyst; butylcatechol prepn catechol alkylation catalyst

IT Beta zeolites  
RL: CAT (Catalyst use); USES (Uses)  
(cobalt-modified; prepn. by catechol alkylation with t-BuOH  
over

Co-beta zeolite catalysts)

IT Alkylation catalysts  
(prepn. by catechol alkylation with t-BuOH over Co-beta  
zeolite  
catalysts)

IT 75-65-0, tert-**Butanol**, reactions 120-80-9, Catechol, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(**catechol** alkylation with t-BuOH over Co-beta **zeolite**  
catalysts)

IT 98-29-3P, 4-tert-Butylcatechol  
RL: IMF (Industrial manufacture); PREP (Preparation)  
(prepn. by catechol alkylation with t-BuOH over Co-beta  
zeolite  
catalysts)

L9 ANSWER 4 OF 7 CA COPYRIGHT 2003 ACS

AN 135:152408 CA

TI Alkylation of dihydroxybenzenes and anisole with  
methyl-tert-butyl ether  
(MTBE) over solid acid catalysts

AU Yadav, G. D.; Goel, P. K.; Joshi, A. V.

CS Chemical Engineering Division, University Department of Chemical  
Technology (UDCT), Matunga, Mumbai, 400 019, India

SO Green Chemistry (2001), 3(2), 92-99  
CODEN: GRCHFJ; ISSN: 1463-9262

PB Royal Society of Chemistry

DT Journal

LA English

CC 22-4 (Physical Organic Chemistry)

AB The synthesis of tert-butylated dihydroxy and alkoxy benzenes  
from

**catechol**, **resorcinol** and anisole, with MTBE has been  
carried out in presence of variety of solid acid catalysts. The  
current  
work dealt with the efficacy of various solid acid catalysts in  
the

alkylation of substituted benzenes and MTBE. MTBE is a better  
tert-butylating agent than **isobutylene** and tert-Bu alc. 20%  
wt./wt. dodecatungstophosphoric acid (DTP) supported on K10  
**montmorillonite** clay was found to be very effective in comparison  
with other solid acid catalysts used. A complete theor. and  
exptl. anal.

is presented for the model studies of **catechol**/anisole with  
MTBE. The reaction follows a typical second order kinetics at a  
fixed

catalyst loading, with weak adsorption of both the species. The  
energy of

activation for **catechol** alkylation was found to be 8.86 kcal mol<sup>-1</sup>, which was low and suggested that intraparticle diffusional resistance would set in for larger particle size. For anisole alkylation

the energy of activation was 17.36 kcal mol<sup>-1</sup> indicating that the reaction

is intrinsically kinetically controlled.

ST dihydroxybenzene anisole alkylation kinetics MTBE solid acid catalysts

IT Reaction kinetics

(Friedel-Crafts reaction kinetics; alkylation of dihydroxybenzenes and

anisole with MTBE over solid acid catalysts)

IT Activation energy

Friedel-Crafts reaction

Friedel-Crafts reaction catalysts

Particle size

Surface reaction

Tert-butylation

(alkylation of dihydroxybenzenes and anisole with MTBE over solid acid

catalysts)

IT Phenols, reactions

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT

(Reactant); PROC (Process); RACT (Reactant or reagent)

(alkylation of dihydroxybenzenes and anisole with MTBE over solid acid

catalysts)

IT Friedel-Crafts reaction

(kinetics; alkylation of dihydroxybenzenes and anisole with MTBE over

solid acid catalysts)

IT 1318-93-0, montmorillonite K10, uses

RL: CAT (Catalyst use); USES (Uses)

(alkylation of dihydroxybenzenes and anisole with MTBE over solid acid

catalysts)

IT 100-66-3, Anisole, reactions 108-46-3, Resorcinol, reactions 120-80-9,

Catechol, reactions

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT

(Reactant); PROC (Process); RACT (Reactant or reagent)

(alkylation of dihydroxybenzenes and anisole with MTBE over solid acid

catalysts)

IT 1634-04-4, MTBE

RL: RCT (Reactant); RACT (Reactant or reagent)

(alkylation of dihydroxybenzenes and anisole with MTBE over solid acid

catalysts)  
IT 1343-93-7  
RL: CAT (Catalyst use); USES (Uses)  
(supported on K10 montmorillonite clay; alkylation of  
dihydroxybenzenes  
and anisole with MTBE over solid acid catalysts)  
RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD  
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L9 ANSWER 5 OF 7 CA COPYRIGHT 2003 ACS  
AN 133:237465 CA  
TI Alkylation of hydroquinone with methyl-tert-butyl-ether and  
tert-butanol  
AU Yadav, G. D.; Doshi, N. S.  
CS University Department of Chemical Technology (UDCT), Chemical  
Engineering  
Division, University of Mumbai, Matunga, Mumbai, 400 019, India  
SO Catalysis Today (2000), 60(3-4), 263-273  
CODEN: CATTEA; ISSN: 0920-5861  
PB Elsevier Science B.V.

*ordered*

DT Journal  
 LA English  
 CC 22-4 (Physical Organic Chemistry)  
 Section cross-reference(s): 45, 67  
 AB The alkylation of **hydroquinone** yields industrially important compds., amongst which tert-butylhydroquinone is a very important precursor for its use in pharmaceuticals and in developing photog. plates.  
 Twenty per cent (wt./wt.) dodecatungstophosphoric acid supported on K10 **montmorillonite** clay (DTP/K10) was found to be a very efficient and novel catalyst in comparison with several others for alkylation of **hydroquinone** with different alkylating agents such as methyl-tert-butyl-ether (MTBE) and tert-**butanol** at 150.degree.C in an autoclave. A summary of characterization of DTP/K10 is provided and related to the activity. Various reaction parameters were also investigated and a kinetic model was built. The rate of alkylation with MTBE was much faster than that with tert-**butanol**. The reaction follows a typical second order kinetics at a fixed catalyst loading with weak adsorption of both the species. The energy of activation was found to be 19.34 kcal/mol.  
 ST alkylation **hydroquinone** MTBE **butanol** heteropoly acid **montmorillonite** clay  
 IT Catalyst supports  
 (K10 **montmorillonite** clay; kinetics and mechanism of alkylation of **hydroquinone** with methyl-tert-Bu ether and tert-**butanol** over solid acid catalysts)  
 IT Activation energy  
 Adsorption  
 Alkylation  
 Alkylation catalysts  
 Alkylation kinetics  
 Surface reaction  
 (kinetics and mechanism of alkylation of hydroquinone with methyl-tert-Bu ether and tert-butanol over solid acid catalysts)  
 IT Heteropoly acids  
 RL: CAT (Catalyst use); USES (Uses)  
 (kinetics and mechanism of alkylation of hydroquinone with methyl-tert-Bu ether and tert-butanol over solid acid catalysts)  
 IT Clays, uses  
 RL: CAT (Catalyst use); USES (Uses)  
 (montmorillonitic, K10; kinetics and mechanism of alkylation of hydroquinone with methyl-tert-Bu ether and tert-butanol over solid acid

catalysts)

IT Acids, uses  
 RL: CAT (Catalyst use); USES (Uses)  
 (solid; kinetics and mechanism of alkylation of hydroquinone  
 with methyl-tert-Bu ether and tert-butanol over solid acid  
 catalysts)

IT 7646-85-7, Zinc dichloride, uses  
 RL: CAT (Catalyst use); USES (Uses)  
 (clayzic (20% ZnCl<sub>2</sub>/K-10 montmorillonite); kinetics and  
 mechanism of alkylation of **hydroquinone** with methyl-tert-Bu  
 ether and tert-**butanol** over solid acid catalysts)

IT 1314-23-4D, Zirconia, sulfated 1343-93-7 12027-38-2  
 RL: CAT (Catalyst use); USES (Uses)  
 (kinetics and mechanism of alkylation of hydroquinone with  
 methyl-tert-Bu ether and tert-butanol over solid acid  
 catalysts)

IT 88-58-4P, 2,5-Di-tert-butyl-1,4-hydroquinone 1948-33-0P,  
 2-tert-Butyl-1,4-hydroquinone  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation);  
 PREP  
 (Preparation)  
 (kinetics and mechanism of alkylation of hydroquinone with  
 methyl-tert-Bu ether and tert-butanol over solid acid  
 catalysts)

IT 123-31-9, p-Hydroquinone, reactions 1634-04-4, MTBE  
 RL: PEP (Physical, engineering or chemical process); PRP  
 (Properties); RCT  
 (Reactant); PROC (Process); RACT (Reactant or reagent)  
 (kinetics and mechanism of alkylation of hydroquinone with  
 methyl-tert-Bu ether and tert-butanol over solid acid  
 catalysts)

IT 75-65-0, tert-Butanol, reactions  
 RL: PEP (Physical, engineering or chemical process); RCT  
 (Reactant); PROC  
 (Process); RACT (Reactant or reagent)  
 (kinetics and mechanism of alkylation of hydroquinone with  
 methyl-tert-Bu ether and tert-butanol over solid acid  
 catalysts)

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- (21) Young, C; Ind Eng Chem Res 1990, V24, P642

L9 ANSWER 6 OF 7 CA COPYRIGHT 2003 ACS

AN 132:207509 CA

TI Alkylation of catechol with t-butyl alcohol over acidic zeolites

AU Yoo, J. W.; Lee, C. W.; Park, S.-E.; Ko, J.

CS Yusung, P.O. Box 107, Industrial Catalysis Research Lab., Korea Research

Institute of Chemical Technology (KRICT), Taejon, S. Korea

SO Applied Catalysis, A: General (1999), 187(2), 225-232

CODEN: ACAGE4; ISSN: 0926-860X

PB Elsevier Science B.V.

DT Journal

LA English

CC 22-4 (Physical Organic Chemistry)

Section cross-reference(s): 67

OS CASREACT 132:207509

AB The catalytic properties of H-ZSM-5 in catechol alkylation with Me3COH are

compared to that of other solid acid catalysts, H-USY, H-beta, .gamma.-alumina. H-ZSM-5 zeolite shows a selectivity >84% and conversion

>90% for 4-tert-butylcatechol (4-TBC), while 3,5-di-tert-butylcatechol

(DTBC) and 3-tert-butylcatechol (3-TBC) are produced as minor byproducts,

which are identified by GC/MS and 1H-NMR. When the Na cation-exchange

level, Na/H, of NaH-ZSM-5 increases, the conversion and DTBC selectivity

decrease rapidly and 3-tert-butylcatechol (3-TBC) selectivity grows. As

the SiO2/Al2O3 ratio of H-ZSM-5 increases, the conversion and DTBC

selectivity decrease. Selectivities for 4-TBC over NaH-ZSM-5 with 3

different Na cation-exchange levels and over ZSM-5 with 3 different

QD SUS. A6 1  
pta

SiO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> ratios are not changed significantly. Surface modification of

H-ZSM-5 via CVD with tetraethylorthosilicate (TEOS) or poisoning with

tributylamine (TBA) leads to the redn. of DTBC selectivity, and simultaneously, to the improvement of 4-TBC selectivity.

Variations of

catalytic activity over ZSM-5 catalysts are compared and discussed in

terms of the concn. and strength of the acid site detd. by FTIR spectroscopy. Strong Bronsted acid sites seem to be responsible for the

t-butylation of catechol.

ST tertbutyl alc alkylation **catechol** acidic **zeolite** catalyst; **tertbutanol** tertbutylation **catechol** acidic **zeolite**

IT Surface acidity

Surface acidity

(Bronsted; alkylation of catechol with t-Bu alc. over acidic zeolites)

IT IR spectroscopy

(Fourier-transform; alkylation of catechol with t-Bu alc. over acidic zeolites)

IT Ultrastable Y zeolites

RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process);

PRP (Properties); PROC (Process); USES (Uses)

(HY; alkylation of catechol with t-Bu alc. over acidic zeolites)

IT Surface acidity

Surface acidity

(Lewis; alkylation of catechol with t-Bu alc. over acidic zeolites)

IT Zeolite NaY

RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process);

PRP (Properties); PROC (Process); USES (Uses)

(NaHZSM-5; alkylation of catechol with t-Bu alc. over acidic zeolites)

IT Catalysis

(acid; alkylation of catechol with t-Bu alc. over acidic zeolites)

IT Zeolites (synthetic), properties

RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process);

PRP (Properties); PROC (Process); USES (Uses)

(acidic; alkylation of catechol with t-Bu alc. over acidic zeolites)

IT Alkylation

Chemisorbed substances

Chemisorption  
 IR spectra  
 Poisoning, catalytic  
 Surface reaction  
 Tert-butylation  
 (alkylation of catechol with t-Bu alc. over acidic zeolites)  
 IT H-Beta zeolites  
 Zeolite ZSM-5  
 RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process);  
 PRP (Properties); PROC (Process); USES (Uses)  
 (alkylation of catechol with t-Bu alc. over acidic zeolites)  
 IT Alcohols, reactions  
 RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)  
 (alkylation of catechol with t-Bu alc. over acidic zeolites)  
 IT Cation exchange  
 (catalyst effect of Na; alkylation of catechol with t-Bu alc. over acidic zeolites)  
 IT Tert-butylation  
 Tert-butylation  
 (catalysts; alkylation of catechol with t-Bu alc. over acidic zeolites)  
 IT Vapor deposition process  
 (chem., catalytic effect of TEOS; alkylation of catechol with t-Bu alc. over acidic zeolites)  
 IT Bronsted acidity  
 Bronsted acidity  
 Lewis acidity  
 Lewis acidity  
 Reaction mechanism  
 (surface; alkylation of catechol with t-Bu alc. over acidic zeolites)  
 IT Alkylation catalysts  
 Alkylation catalysts  
 (tert-butylation; alkylation of catechol with t-Bu alc. over acidic zeolites)  
 IT Zeolite HY  
 RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process);  
 PRP (Properties); PROC (Process); USES (Uses)  
 (ultrastable; alkylation of catechol with t-Bu alc. over acidic zeolites)  
 IT 78-10-4, Tetraethylorthosilicate  
 RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process);

PROC (Process); USES (Uses)  
 (CVD of zeolite catalyst; alkylation of catechol with t-Bu alc. over acidic zeolites)

IT 1020-31-1P, 3,5-Di-tert-butylcatechol 4026-05-5P,  
 3-tert-Butylcatechol  
 RL: BYP (Byproduct); PREP (Preparation)  
 (alkylation of catechol with t-Bu alc. over acidic zeolites)

IT 75-65-0, tert-Butyl alcohol, reactions 120-80-9,  
 1,2-Benzenediol, reactions  
 RL: PEP (Physical, engineering or chemical process); RCT  
 (Reactant); PROC  
 (Process); RACT (Reactant or reagent)  
 (alkylation of catechol with t-Bu alc. over acidic zeolites)

IT 98-29-3P, 4-tert-Butylcatechol  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (alkylation of catechol with t-Bu alc. over acidic zeolites)

IT 102-82-9, Tributylamine  
 RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process);  
 PROC (Process); USES (Uses)  
 (catalyst poison; alkylation of catechol with t-Bu alc. over acidic zeolites)

IT 7440-23-5, Sodium, uses  
 RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process);  
 PROC (Process); USES (Uses)  
 (catalytic effect of zeolite cation exchange; alkylation of catechol with t-Bu alc. over acidic zeolites)

IT 110-86-1, Pyridine, properties  
 RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process);  
 PRP (Properties); PROC (Process); USES (Uses)  
 (chemisorption; alkylation of catechol with t-Bu alc. over acidic zeolites)

IT 1344-28-1, Alumina, properties  
 RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process);  
 PRP (Properties); PROC (Process); USES (Uses)  
 (.gamma.-; alkylation of catechol with t-Bu alc. over acidic zeolites)

RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD  
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COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
56.61	58.42

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-5.58	-5.58

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